MTE-20

Process Modelling of A PVC Production Plant

Chan Jun Hoa[1] Dominic C. Y. Foo[2] Sivakumar Kumaresan[1]
Ramlan Abdul Aziz[1] Mohd Ariffin Abu Hassan[3]

[1] *Chemical Engineering Pilot Plant, Universiti Teknologi Malaysia*
81310 Skudai, Johor, Malaysia.
Tel: +60-7-553-1662, Fax: +60-7-556-9706, E-mail: shiva@cepp.utm.my; ramlan@cepp.utm.my

[2] *School of Chemical and Environmental Engineering, University of Nottingham (Malaysia Campus)*
Jalan Broga 43500 Semenyih Selangor Darul Ehsan Malaysia.
Tel: +60-3-8924-8130, Fax: +60-3-8924-8017, E-mail: Dominic.Foo@nottingham.edu.my

[3] *Chemical Engineering Department, Universiti Teknologi Malaysia*
81310 Skudai, Johor, Malaysia.
Tel: +60-7-553-5485, Fax: +60-7-558-1463, E-mail: m.ariffin@fkkksa.utm.my

Abstract

This paper presents the modelling of a Polyvinyl Chloride (PVC) resins manufacturing process with batch process simulator, SuperPro Designer V6.0. The simulation model has been developed based on the operating condition of a local PVC manufacturing plant. As the polymerisation process is carried out in batch operation mode, efforts have been made to document the scheduling details of each unit operation and results are presented in the Gantt chart. Cycle time for a complete polymerisation process is determined to be 14.28 hours. The model also reveals that approximately 17 batches of polymerisation reaction can be processed per day, which tallies the real operation of the PVC manufacturing plant.

Keywords: Modelling, optimisation, batch process, scheduling, PVC production.

Introduction

The Computer Aided Process Design (CAPD) and simulation tools have been widely used in the bulk and petrochemical industries since the early 1960's. It involves the use of computers to perform steady-state heat and mass balancing as well as sizing and costing calculations for a process [1]. However, the use of these CAPD and simulation tools has only emerged in the batch manufacturing in the past decade [2-7]. Compared to the readily available commercial process simulators in the bulk chemical industries, there are only a limited number of commercial simulators available for batch process modelling in the market, which include Batches by Batch Process Technologies, Batch Plus by Aspen Technology, SuperPro Designer by Intelligen as well as Batch Design Kit by Hyprotech. This situation is mainly due to the complexity associated with batch processes that are frequently operated in cyclical mode. Due to its relatively new emergence, much work needs to be done in this sector.

This paper describes the use of the commercial batch process simulator SuperPro Designer v6.0 [8] in the modelling of a local industrial production of polyvinyl chloride (PVC), which is operated in mixed batch and continuous mode.

PVC Manufacturing Case Study

Figure 1 shows the process flow diagram of the PVC resins manufacturing. It consists of 10 parallel batch polymerisation reactors, blow-down vessel, and two parallel trains of downstream processing equipment. Each downstream processing train consists of a stripper, two decanters and a fluid bed dryer. The plant is operated in a semi-batch mode where upstream reactors are scheduled to match the downstream processing trains that are operated in continuous mode.

The batch reactor feed consist of a mixture of fresh vinyl chloride monomer (VCM) and recycled VCM from the process, mainly from blowdown vessel and stripper. At the polymerising or reaction section of the plant, the polymerising process is carried out subsequently in ten parallel batch reactors. Raw materials for the polymerisation process include demineralised water, VCM, initiators and suspending agents. These raw material are charged into the reactor in sequence. The pH of the deionised water is kept between 6.6 – 9.0. The suspending agent is diluted to approximately 4.0wt% and is charged into the reactor together with demineralised water. This is mainly due to the high viscosity of the suspending agent solution.

Upon the completion of suspending agent charge, primary and secondary initiators are added into the reactor manually via the vessel man hole. Manual charging of initiator is

required as fluctuations resulted from the automated charging system may lead to severe safety problem is not tolerable. Two types of initiators are used in this polymerisation process, with the primary initiator in powder form while the secondary initiator in flakes form.

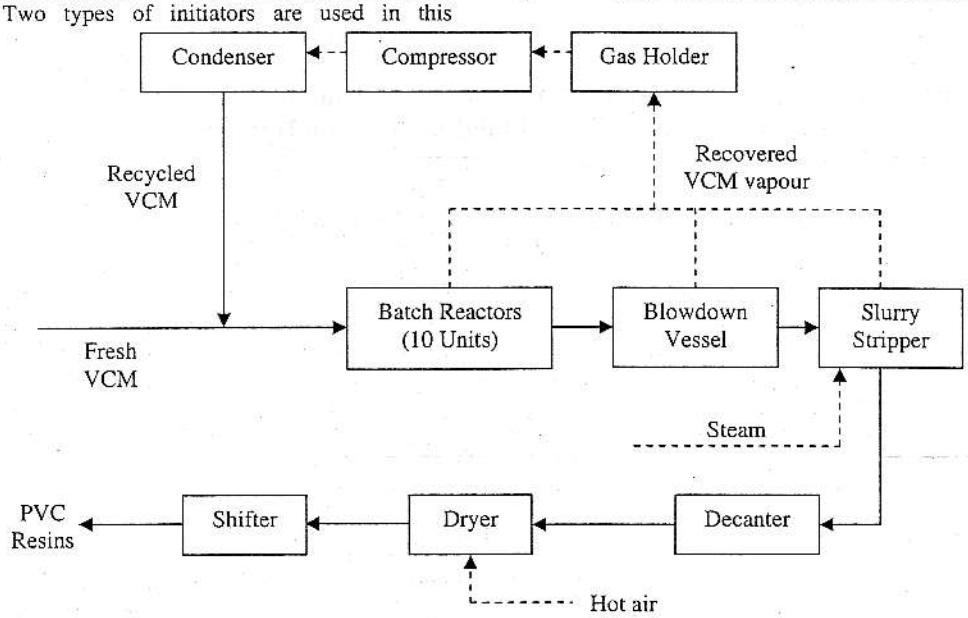


Figure 1 – Process flow diagram of a PVC manufacturing plant

The batch reactor feed consist of a mixture of fresh vinyl chloride monomer (VCM) and recycled VCM from the process, mainly from blowdown vessel and stripper. At the polymerising or reaction section of the plant, the polymerising process is carried out subsequently in ten parallel batch reactors. Raw materials for the polymerisation process include demineralised water, VCM, initiators and suspending agents. These raw material are charged into the reactor in sequence. The pH of the deionised water is kept between 6.6 – 9.0. The suspending agent is diluted to approximately 4.0wt% and is charged into the reactor together with demineralised water. This is mainly due to the high viscosity of the suspending agent solution.

Upon the completion of suspending agent charge, primary and secondary initiators are added into the reactor manually via the vessel man hole. Manual charging of initiator is required as fluctuations resulted from the automated charging system may lead to severe safety problem is not tolerable. Two types of initiators are used in this polymerisation process, with the primary initiator in powder form while the secondary initiator in flakes form.

It shall also be noted that, due to piping constrain, demineralised water can only be charged into the reactors one at a time. Demineralised water charging in each reactor takes approximately 20 minutes to complete. Charging procedure in each of the reactor will only start after the end of charging in an earlier reactor. The same situation occurs to the charging of VCM and the blowdown operation after the reaction ends.

After the charging of water completes, the reactor is purged by nitrogen and then vacuumed before charging of VCM is charged. This is to ensure that no oxygen is present in the reactor as reaction between VCM and oxygen and might result in explosion.

Upon the completion of VCM charge, heating is commence to raise the reactor temperature to the optimal reaction temperature of 57°C and a working pressure of 8.9 bar. Exothermic polymerisation process next commences, for a duration of 7.5 hours. Continuous cooling is needed to remove excess heat and to maintain the reactor temperature at 57°C. PVC polymer is the main product at the end of the polymerisation process. Other by-products of the reaction are the unreacted VCM, initiators, suspending agent and some trace amount of contaminant. The reactor content is now present in slurry form (a mixture of PVC and water) and is ready to be sent to the blowdown system.

The blowdown vessel receives batches of slurry which are intermittently discharged from the reactors. The blowdown vessel acts as buffer storage so that slurry can be continuously fed to the two parallel downstream processing trains. As slurry is discharged from the reactor, large lumps which could block downstream equipment are removed by strainers. As the slurry enters the blowdown vessel, the major portion of the unreacted VCM trapped in the PVC particles flashes of and is vented to the gasholder for recovery. The VCM vapour is next compressed and condensed into liquid form before it is reused in the polymerisation process.

As the effluent from the blowdown vessel enters the downstream processing trains, the stripper column further

removes the unreacted VCM from the PVC slurry. Steam is introduced at the base of the stripping column and the VCM is removed as an overhead product to the gasholder. The stripped slurry is then directed to two parallel decanters for water removal. Approximately 79% of water is removed by these decanters from the PVC slurry

Wet cake from the decanters is next sent to the fluidised bed dryer to be dried by hot air and hot water (in tubes which are heated by steam). Direct usage of steam in the dryer is not practical as the PVC resins have a low Glass Transition Temperature (T_g) of 78°C. Exposure of PVC resins under the steam of 100°C will cause the structure of the resins to collapse. This softens the PVC resins and results in poor quality of resins.

Dried PVC resins are transported by cool plant air to the shifter. The use of cool plant air avoids the electrostatic force that may cause the resins to flocculate. Fine resins that pass through the shifter (60 mesh) are sold as product while the course resins are grinded and sold as low-grade resins.

Base Case Process Simulation

Figure 2 shows the base case process simulation model that has been developed based on the operating condition of the PVC manufacturing process using SuperPro Designer V6.0 (Intellegen, 2005). The annual operating time of the process model is taken as 7920 hours.

In the modelling environment of SuperPro Designer, a few *operations* take place sequentially in a single *unit procedure* (Intellegen, 2005). For instance, vessel procedure P-1 in Figure 2 is used to model the batch polymerisation process that consist of sequential operations of raw material charges, vacuum, material heating, polymerisation process as well as product blowdown. All these individual operations take place in vessel K207 (where vessel procedure P-1 takes place). The modelling of these single operations is described next.

The raw material charged into K207 during the start of procedure P-1 includes demineralised water (CHARGE-H2O), suspending agent (CHARGE-PVA), primary initiator (CHARGE-CAT1) and secondary initiator (CHARGE-CAT2). Properties of the raw materials used in the model are summarised in Table 1. Note that suspending agent, primary and secondary initiators are user defined components where their properties have been changed in the model. Note that the model has included the actual operating condition of the PVC manufacturing process, where the charging of demineralised water for a subsequent reactor is scheduled to start after the water charging of the preceding reactor ends. Suspending agent, primary and secondary initiators are charged into the reactor during the charging of water.

The vacuum operations (VACUUM) in procedure P-1 include a vacuum air purge from the reactor to 0.226 atm (gauge pressure = -0.8 kg/cm^2) followed by a nitrogen gas purge to 1.194 atm (gauge pressure = 0.2 kg/cm^2) and another vacuum purge to 0.226 atm (gauge pressure = -0.8 kg/cm^2). The vacuum operations were carried out before the charging of VCM (CHARGE-VCM). This is to avoid the mixing of VCM with air, which might lead to explosion.

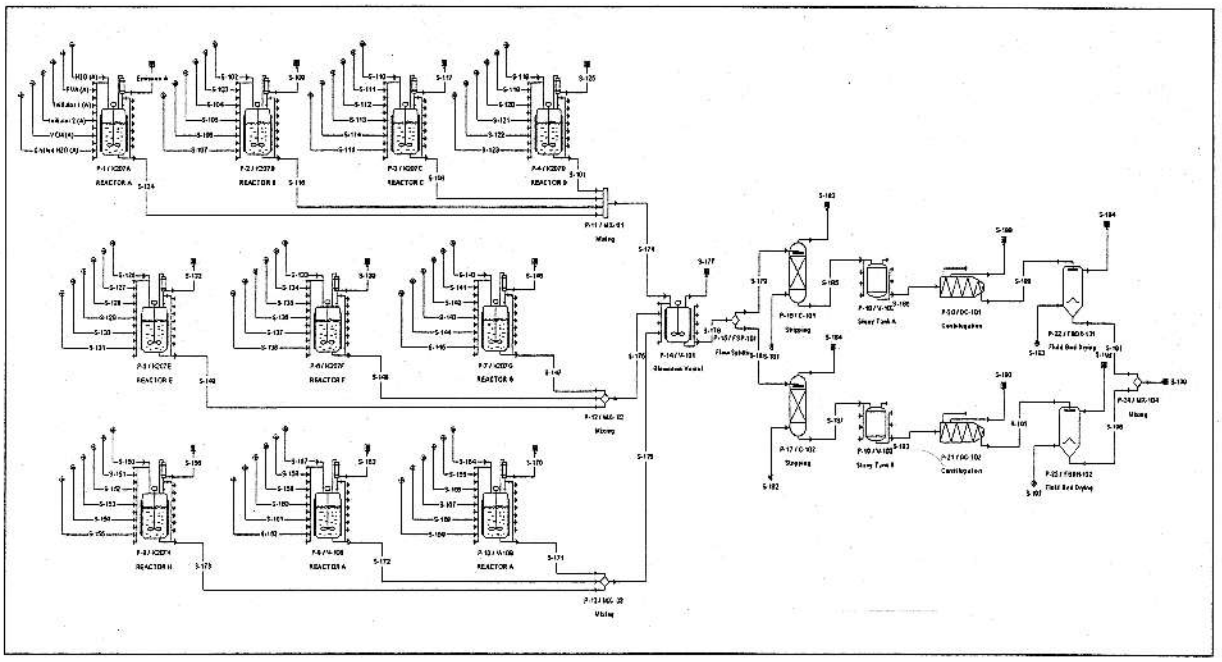


Figure 2 – Simulation flowsheet of PVC manufacturing

Table 1 - Feed Stream Specification

Component	Amount/reactor	Property
Chilled H_2O	300 US gal (1135.62 kg)	User defined (referred to water)
Primary initiator	3.7 kg	MW = 571.00
Secondary initiator	0.7 kg	MW = 398.70 Normal boiling point = 467 °C Melting point = 48 °C
Suspending agent	155 kg	Melting point = 228 °C
VCM	7700 kg	SuperPro Database
Water	10500 kg	SuperPro Database

In the heating operation, hot water (inlet temperature of 90°C and outlet temperature of 70°C) is defined as a new heat transfer agent to heat the reactor to 57 °C where polymerisation process (REACT-1) occurs. In the reaction operation, duration of the polymerisation process takes 7.5 hours and the reaction extent is set at 90%. Stoichiometric reaction model is used and the reaction stoichiometric is defined to convert one mass of VCM to one mass of PVC, as follow:

$$n(\text{VCM}) \rightarrow (\text{PVC})_n \qquad (1)$$

The last operation in the vessel procedure is to discharge (TRANS-OUT) the slurry reactor content to the blowdown procedure P-14 (in vessel V-101). Similar to the case of demineralisation water charge, blowdown operation of a subsequent reactor is also scheduled to start after the completion a preceding reactor, due to the piping constrain in the actual process. The specification of the process vessels is shown in Table 2.

Table 2 – Equipment Specification Table

Equipment	Equipment tag	Volume (m^3)
Polymerisation reactors	K207A-K207J	20
Blowdown vessel	V-101	94
Slurry tank	V-12 and V-13	100

As the polymerisation process is carried out in batch operation mode, efforts have been made to document the scheduling details for each of the batch vessel procedure (P-1 to P-10). This includes the *setup time* (SUT), *process time* (PT), and *start time* (ST) of each individual operation in the vessel procedure. The details of this scheduling summary are shown in Table 3, with the process Gantt chart shown in Figure 3.

From the blowdown vessel, the slurry product enters into two parallel identical downstream processing trains which individually consist of a stripper, slurry tank, two parallel identical decanters and a fluid-bed dryer that operate in continuous mode. Thus, no scheduling is needed in these processes. The modelling specifications of each unit procedure in these downstream processing trains are next described.

Stripper procedures (P-16 and P-17) are used for VCM removal. The design component of the strippers is selected to be VCM. 2880 kg of steam at 110°C is introduced to the stripper to achieve a VCM removal of 99.9%. In the simulation model, the condenser at the stripper top which condenses the steam is omitted since VCM recovery facility in not modelled. Hence, the steam leaves as emission together with VCM. This leads to a slight decrease in the total amount of wastewater discharged from the decanter, which however can be omitted due to its insignificant amount.

The slurry tanks (P-17 and P-18) serve as temporary storage for the PVC slurry before it enters into the two parallel identical decanters (P-20 and P-21; not shown in Fig 3.2). Solid removal in the decanters is specified as 99% for PVC, with water lost of 21% (include chilled water lost). Effluent emits from these decanter units is the main wastewater of the process; while the wet filter cake is sent to fluidised-bed dryers for moisture removal.

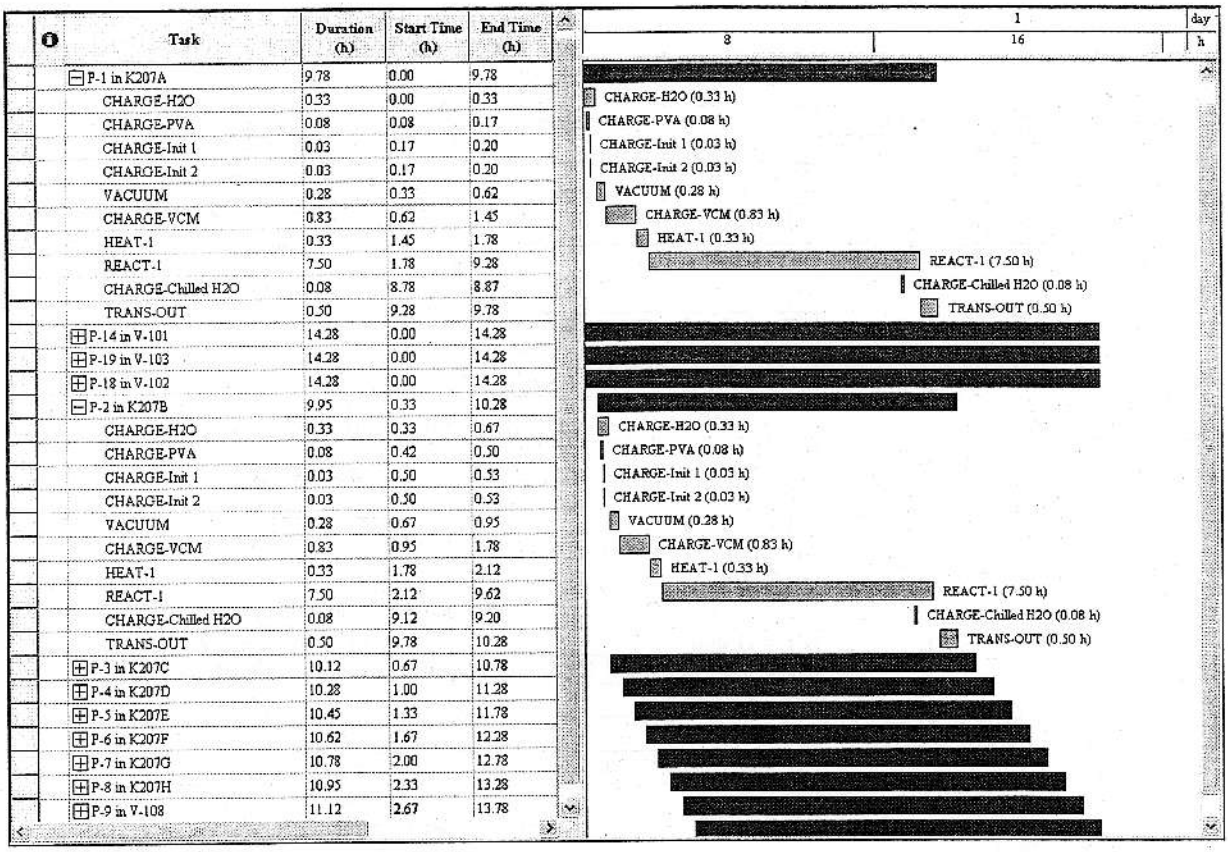
In the fluidised-bed dryers (P-22 and P-23), hot air at 95 °C is used to dry the wet filter cake. Evaporation rate of water and the final solid temperature are set at 916 kg H_2O /h and 60°C respectively. As a result, 99.8% of the moisture (the component of water and chilled water) is removed.

From the simulation model, the cycle time for a complete batch polymerisation process is 14.28 hours. This model also reveals that approximately 17 batches of polymerisation reaction can be processed per day, which tallies the real operation of the PVC manufacturing plant. Based on the annual operating time of 7920 hours, this translates into 554 batches/year.

It should also be noted that, all vessel procedures (P-1 to P-10) are observed to have different cycle time (see Gantt Chart in Figure 3). This is mainly due to the scheduling of the TRANSFER-OUT-1 operations in each of the reactor procedures (P-1 to P-10). Since TRANSFER-OUT-1 operation in each of the reactor is scheduled to start after the TRANSFER-OUT-1 operation of the preceding reactor ends, this creates a lag time for the product to be discharged from the subsequent reactor before the preceding reactor completes its TRANSFER-OUT-1 operation. A good example is shown in Figure 3. As shown, the polymerisation reaction in P-2/K-207B completed at 9.62 hr. However, due to the TRANSFER-OUT-1 of P-1/K-207A is in operation, TRANSFER-OUT-1 operation in P-2/K-207B cannot start until the TRANSFER-OUT-1 operation in P-1/K-207A ends at 9.78 hr. Hence, this leads to a lag time of 0.16 hr.

Table 3 – Scheduling Summary for Base Case Simulation

Procedure	Operation	Process scheduling	Remarks
P-1/K207A to P-10/K207J	Charge in Demineralised Water (CHARGE-H2O)	SUT = 0 min	CHARGE-H2O for second and subsequent reactor starts after the end of CHARGE-H2O in preceding reactor
		PT = 20 min	
		ST = Beginning of batch	
	Charge in Suspending Agent (CHARGE-PVA)	SUT = 0 min	
		PT = 5 min	
		ST = 5min after CHARGE- H2O starts	
	Charge in Primary Initiator (CHARGE-CAT1)	SUT = 0 min	Charged in manually
		PT = 2 min	
		Start time = 10 min after CHARGE-H2O starts	
	Charge in Secondary Initiator (CHARGE-CAT2)	SUT = 0 min	Charged in manually
		PT = 2 min	
		Start time = 10 min after CHARGE-H2O starts	
	Vacuum (VACUUM)	SUT = 0 min	First Vacuum to 0.226 atm
		PT = 17 min	Purge with N_2 to 1.194 atm
		ST = After CHARGE-H2O ends	Second Vacuum to 0.226 atm
	Charge in VCM (CHARGE-VCM)	SUT = 5 min	Valve opening and pump switching carried out manually
		PT = 45 min	
		ST = after VACUUM ends	
	Heat (HEAT-1)	SUT = 0 min	Use hot water (90 - 70°C) as heating agent
		PT = 20 min	Final heating T = 57°C
		ST = after CHARGE-VCM ends	
	Polymerisation (REACT-1)	SUT = 0 min	Reaction T = 57°C
			Reaction P = 8.9 bar
		PT = 450 min	$\Delta H_{reaction}$ = -367.7 kcal/kg
			Emission = 20% of VCM (off vent condenser)
		ST= After HEAT-1 ends	Conversion = 90%
			Cooling agent = cooling water at 25°C
	Charge in Chilled Water (CHILLED H20)	SUT = 0 min PT = 5 min ST = 7 h after REACT-1 starts	
	Blowdown (TRANSFER-OUT-1)	SUT = 0 min	Scheduled to start after the transfer out of previous reactor ends
		PT = 30 min	
		ST= after REACT-1 ends	



Task	Duration (h)	Start Time (h)	End Time (h)
P-1 in K207A	9.78	0.00	9.78
CHARGE-H2O	0.33	0.00	0.33
CHARGE-PVA	0.08	0.08	0.17
CHARGE-Init 1	0.03	0.17	0.20
CHARGE-Init 2	0.03	0.17	0.20
VACUUM	0.28	0.33	0.62
CHARGE-VCM	0.83	0.62	1.45
HEAT-1	0.33	1.45	1.78
REACT-1	7.50	1.78	9.28
CHARGE-Chilled H2O	0.08	8.78	8.87
TRANS-OUT	0.50	9.28	9.78
P-14 in V-101	14.28	0.00	14.28
P-19 in V-103	14.28	0.00	14.28
P-18 in V-102	14.28	0.00	14.28
P-2 in K207B	9.95	0.33	10.28
CHARGE-H2O	0.33	0.33	0.67
CHARGE-PVA	0.08	0.42	0.50
CHARGE-Init 1	0.03	0.50	0.53
CHARGE-Init 2	0.03	0.50	0.53
VACUUM	0.28	0.67	0.95
CHARGE-VCM	0.83	0.95	1.78
HEAT-1	0.33	1.78	2.12
REACT-1	7.50	2.12	9.62
CHARGE-Chilled H2O	0.08	9.12	9.20
TRANS-OUT	0.50	9.78	10.28
P-3 in K207C	10.12	0.67	10.78
P-4 in K207D	10.28	1.00	11.28
P-5 in K207E	10.45	1.33	11.78
P-6 in K207F	10.62	1.67	12.28
P-7 in K207G	10.78	2.00	12.78
P-8 in K207H	10.95	2.33	13.28
P-9 in V-108	11.12	2.67	13.78

Figure 3 – Process Gantt Chart for Base Case Simulation

Conclusion

A simulation model based on the operating condition of a PVC manufacturing process has been developed on a batch process simulation software. The developed model tallies the real operation where 17 batches of polymerisation process are carried out per day. This translates into 554 batches of product per annum.

Acknowledgement

The technical support of Mr Yoeng Chee Nyok of Industrial Resin (Malaysia) Berhad is gratefully acknowledged.

References

[1] Westerberg, A. W., Hutchison, H. P., Motard, R. L. and Winter, P. 1979. *Process Flowsheeting*. Cambridge: Cambridge University Press.

[2] Petrides, D., Sapidou, E. and Calandranis, J. 1995. Computer-aided Process Analysis and Economic Evaluation for Biosynthetic Human Insulin Production - A Case Study. *Biotechnology and Bioengineering* 48: 529-541.

[3] Hwang, F. 1997. Batch Pharmaceutical Process Design and Simulation. *Pharmaceutical Engineering* January/February 1997: 28-43.

[4] Ernst, S., Garro, O. A., Winkler, S., Venkataraman, G., Langer R., Cooney, C. L. and Sasisekharan, R. 1997. Process Simulation for Recombinant Protein Production: Cost Estimation and Sensitivity Analysis for Heparinase I Expressed in *Escherichia coli*. *Biotechnology and Bioengineering* 53(6): 575-582.

[5] Koulouris, A., Calandranis, J. and Petrides, D. P. 2000. Throughput Analysis and Debottlenecking of Integrated Batch Chemical Processes. *Computers and Chemical Engineering* 24: 1387-1394.

[6] Petrides, D. P., Koulouris, A. and Siletti, C. 2002. Throughput Analysis and Debottlenecking of Biomanufacturing Facilities: A Job for Process Simulators. *BioPharm* August 2002: 2-7.

[7] Petrides, D. P., Koulouris, A. and Siletti, C. 2002. The Role of Process Simulation in Pharmaceutical Process Development and Product Commercialization. *Pharmaceutical Engineering* 22(1): 56-65.

[8] Oh, S. K. W., Kuek, K. H. and Wong, V. V. T. 2004. Design, Simulation and Optimisation of A Large Scale Monoclonal Antibody Production Plant: Upstream Design. *Pharmaceutical Engineering* 24(6): 42-60.

[9] Intelligen, Inc. 2005. *SuperPro Designer User's Guide*, Scotch Plains: Intelligen, Inc.